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AND KERNELS FOR LIQUID PARA- AND ORTHO-HYDROGEN

by

Y. D. Naliboff

prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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TOPICAL REPORT

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July 30, 1964

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Technical Management
NASA-Lewis Research Center
Advanced Development and Evaluation Division
Michael J. Kolar

The LHK computer code is described herein as it existed on July 30, 1964. The code has been in continuous development for 1 year and in its presented form has been applied successfully by General Atomic to the kind of problems discussed later in this report. However, the development and improvement of the code are being continued, so that duplication of results (or even close agreement) between problems run with the code as published and the code as it existed either before or after this time is not necessarily to be expected.

General Atomic has exercised due care in preparation, but does not warrant the merchantability, accuracy, and completeness of the code or of its description contained herein. The complexity of this kind of program precludes any guarantee to that effect. Therefore, any user must make his own determination of the suitability of the code for any specific use, and of the validity of the information produced by use of the code.

INTRODUCTION

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This report describes the code LHK, which calculates double-differential cross sections, total cross sections, and kernels for liquid para- and ortho-hydrogen. The physical model and derivation of the equations are given in reference (1).

Section I presents the equations as they are used in the code; Section II provides an over-all description of the code and comments about various subroutines; III discusses the various approximations used, their effects, and some of the checks made; IV describes additions to the code which may be made; and Section V gives the input instructions.

Fuller

I. The Equations

The equations given here are those of reference (1) rewritten so that subscripts number from one up, rather than from 0, for ease in programming. Some simple regrouping has been done, again for convenience.

$$\frac{d^2\sigma}{dE d\Omega}|_{\text{para}} = \sigma_P(E, E_0, \mu) = \sqrt{\frac{E}{E_0}} \sqrt{\frac{m}{\pi \hbar^2 \kappa^2 kT}} \sum_{n=1}^5 \frac{1}{(n-1)!} \left(\frac{\hbar^2 \kappa^2}{4m} \right)^{n-1} \cdot \left\{ \sum_{l=1,2,\dots} a_l^P (2l-1) \exp \left[-(\epsilon + E_l + (n-1)\omega + \frac{\kappa^2 \hbar^2}{4m})^2 / \left(\frac{\hbar^2 \kappa^2 kT}{m} \right) \right] |A_{n,l}|^2 \right\} \quad (1)$$

$$\frac{d^2\sigma}{dE d\Omega}|_{\text{ortho}} = \sigma_O(E, E_0, \mu) = \sqrt{\frac{E}{E_0}} \sqrt{\frac{m}{\pi \hbar^2 \kappa^2 kT}} \sum_{n=1}^5 \frac{1}{(n-1)!} \left(\frac{\hbar^2 \kappa^2}{4m} \right)^{n-1} \cdot \left\{ \sum_{l=1,2,\dots} a_l^{\text{or}} \exp \left[-\left(\epsilon + E_l - E_2 + (n-1)\omega + \frac{\kappa^2 \hbar^2}{4m} \right)^2 / \left(\frac{\hbar^2 \kappa^2 kT}{m} \right) \right] \cdot \left[l |A_{n,l+1}|^2 + (l-1) |A_{n,l-1}|^2 \right] \right\}, \quad (2)$$

where

$$a_l^P = \begin{cases} a_c^2 & l = 1, 3, 5, \dots \\ a_i^2 & l = 2, 4, 6, \dots \end{cases} \quad a_l^{\text{or}} = \begin{cases} a_i^2/3 & l = 1, 3, 5, \dots \\ a_c^2 + \frac{2}{3} a_i^2 & l = 2, 4, 6, \dots \end{cases}$$

$$E_l = \frac{.014712}{2} l(l-1), E_1 = .014712, \kappa^2 = \frac{2m}{\hbar^2} (E_0 + E - 2\mu \sqrt{EE_0}),$$

$$\epsilon = E - E_0, A_{n,l} = A_{n,l}^{\pm} \left(\alpha = \frac{\kappa a}{2}, \lambda = \frac{\hbar^2 \kappa^2}{8m\omega} \right).$$

When $\kappa^2/8M\omega \ll 1$, the simpler expressions below may be used:

$$\sigma^P(E, E_0, \mu) = 4 \sqrt{\frac{E}{E_0}} \sqrt{\frac{m}{\pi \hbar^2 \kappa^2 kT}} \sum_{l=1,2,\dots} a_l^P (2l-1) \exp \left[- \left(\epsilon + E + \frac{\hbar^2 \kappa^2}{4m} \right)^2 / \left(\frac{\hbar^2 \kappa^2 kT}{m} \right) \right] . \quad (1a)$$

$$. j_l^2 \left(\frac{\kappa a}{2} \right),$$

$$\sigma^{or}(E, E_0, \mu) = 4 \sqrt{\frac{E}{E_0}} \sqrt{\frac{m}{\pi \hbar^2 \kappa^2 kT}} \sum_{l=1,2,\dots} a_l^{or} \exp \left[- \left(\epsilon + E - E_0 + \frac{\hbar^2 \kappa^2}{4m} \right)^2 / \left(\frac{\hbar^2 \kappa^2 kT}{m} \right) \right] .$$

$$. \left[l j_{l+1}^2 \left(\frac{\kappa a}{2} \right) + (l-1) j_{l-1}^2 \left(\frac{\kappa a}{2} \right) \right] , \quad (2a)$$

where the $j_l(\alpha)$ are the spherical bessel functions defined by

$$j_0(x) = \frac{\sin(x)}{x}, j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x}, j_{l+1}(x) = \frac{2l+1}{x} j_l(x) - j_{l-1}(x) . \quad (3)$$

Here, E_0 = initial neutron energy, E = final neutron energy, $\mu = \vec{\Omega} \cdot \vec{\Omega}'$,
 $m = 1.67243 \times 10^{-24}$ gm, $a = 0.75 \times 10^{-8}$ cm, $\hbar^2 = 0.433192 \times 10^{-30}$ (ev·sec)²,
 and kT = liquid hydrogen temperature in ev.

The $A_{n,l}^{\pm}$, are defined by

$$A_{oo}^+ = \int_{-1}^1 d\mu \cos(\alpha\mu) e^{-\lambda\mu^2} \quad (4)$$

$$A_{01}^{-} = \frac{-1}{\lambda} e^{-\lambda} \sin \alpha + \frac{\alpha}{2\lambda} A_{00}^{+}$$

$$A_{02}^{+} = \frac{-3}{2\lambda} e^{-\lambda} \cos \alpha + \left(\frac{3}{2\lambda} - 1\right) \frac{A_{00}^{+}}{2} - \frac{3\alpha}{4\lambda} A_{01}^{-},$$

recursively for higher l by

$$A_{0,l+2}^{-} = \frac{2l+1}{2\lambda(l+2)(2l-1)} \left[(2l-1)(2l+3) + 2\lambda \right] A_{0l}^{-} - \frac{2l+3}{2\lambda(l+2)} \alpha \left[A_{0,l-1}^{+} - A_{0,l+1}^{+} \right] \\ + \frac{(2l+3)(l-1)}{(l+2)(2l-1)} A_{0,l-2}^{-} \quad l = 1, 3, 5, \dots$$

$$A_{0,l+2}^{+} = \frac{2l+1}{2\lambda(l+2)(2l-1)} \left[(2l-1)(2l+3) + 2\lambda \right] A_{0l}^{+} + \frac{(2l+3)}{2\lambda(l+2)} \alpha \left[A_{0,l-1}^{-} - A_{0,l+1}^{-} \right] \quad (5) \\ + \frac{(2l+3)(l-1)}{(l+2)(2l-1)} A_{0,l-2}^{+} \quad l = 2, 4, 6, \dots$$

and, for $n > 0$,

$$A_{n,l}^{\pm} = \frac{l+1}{2l+1} A_{n-1,l+1}^{\mp} + \frac{l}{2l+1} A_{n-1,l-1}^{\mp}$$

Here

$$\alpha = \frac{\kappa a}{2}, \quad \lambda = \frac{\hbar^2 \kappa^2}{4m\nu}.$$

λ and α are used independently in the code although they are related; the choice of which to use is made for convenience.

These recursion relations break down at high ℓ for $\lambda \leq 2$

where the following expansion is used:

$$Q_{0,\ell}^+ = 2i^\ell j_\ell(\alpha) \quad \ell = 0, 2, 4, \dots \quad \left(\text{or } Q_{0,\ell}^+ = 2(-1)^{\ell/2} j_\ell(\alpha) \right)$$

$$Q_{0,\ell}^- = 2i^{\ell-1} j_\ell(\alpha) \quad \ell = 1, 3, 5, \dots \quad \left(\text{or } Q_{0,\ell}^- = 2(-1)^{\frac{\ell-1}{2}} j_\ell(\alpha) \right) \quad (7)$$

$$Q_{n,\ell}^\pm = \frac{\ell+1}{2\ell+1} Q_{n-1,\ell+1}^\mp + \frac{\ell}{2\ell+1} Q_{n-1,\ell-1}^\mp$$

$$\text{and } A_{n,\ell}^\pm = \sum_v \frac{(-\lambda)^v}{v!} Q_{2v+n,\ell}^\pm$$

In the code, the $A_{n,\ell}$ are rewritten so that n and ℓ run from 1 up rather than from 0. Then, $A_{n,\ell}^+$ is used if $\ell+1$ is even, and $A_{n,\ell}^-$ if $\ell+1$ is odd.

II. Code Description

The overall structure of the code is borrowed from a General Atomic code for the calculation of Nelkin water kernels. This code is undocumented, but an intermediate version is described in reference (2).

Given a set of energies and angles, the code calculates the double-differential cross sections for selected energy pairs (those corresponding to down-scattering), integrates over angle to form the Legendre moments (the kernels), forms the upscattering half of the scattering matrix by detailed balance, and finally integrates over final energies to form total cross sections.

The double-differential cross sections for both para- and ortho-hydrogen are produced at the same time by subroutine LHK (Eqs. (1) and (2)) using subroutine CC to evaluate the $A_{n,l}^{\pm}$ (Eqs. (4), (5), (6) and (7)), or, for $\kappa^2/8m\omega \ll 1$, subroutine LHL/W (Eqs. (1a) and (2a)) using CSB for the $j_l(\alpha)$ (eq. (3)).

The angular integration was a matter of some concern. Plots of $\sigma(E, E_0, \mu)$ indicated that a fixed set of angles probably did not produce very reliable kernels and total cross sections. A double-gaussian integration routine was inserted to avoid this difficulty. The code varies the energies as follows: for a fixed initial energy E_0 , final energies are chosen from E_0 down to E_{\min} , the lowest energy in the list. Inspection of angular plots of $\sigma(E, E_0, \mu)$ as E goes from E_0 to E_{\min} indicates that the function is sharply peaked toward $\mu = +1$ for $E_0 \approx E$, and becomes fairly smooth in angle as $E \rightarrow E_{\min}$, with the peak moving smoothly if the energy variation is made in small increments. The ranges for the double-gaussian quadrature are therefore chosen so: for $E = E_0$, the interval $(-1, 1)$ is split at 0.9 into two ranges, $(-1, .9)$ and $(.9, 1)$. Thereafter, for a fixed E_0 , the peak of the angular variation of $\sigma_p(E_i, E_0, \mu)$ is used for the split angle, θ , for the quadrature for the next lower energy, $\sigma_p(E_{i-1}, E_0, \mu)$. The double-range formula for a split angle θ , where w_i and μ_i are weights and abscissae for the interval $(-1, 1)$,

$$\int_{-1}^1 f(x) dx = \sum_{i=1}^N w_i f(\mu_i), \quad \sum_{i=1}^N w_i = 1,$$

is given by

$$\int_{-1}^{\theta} f(x) dx + \int_{\theta}^1 f(x) dx = \sum_{i=1}^N \left\{ \frac{1+\theta}{2} w_i \cdot f\left(\mu_i \frac{1+\theta}{2} + \frac{\theta-1}{2}\right) + \frac{1-\theta}{2} w_i \cdot f\left(\mu_i \frac{1-\theta}{2} + \frac{1+\theta}{2}\right) \right\}. \quad (8)$$

The spherical bessel functions (Eqs. (3)) are calculated in the subroutine CSB by a backward recursion technique⁽³⁾ to avoid numerical difficulties encountered in some ranges of the argument when using the direct approach. In this method, $j_n(\alpha)$ is set to 0, $j_{n-1}(\alpha)$ to an arbitrary small number (say 10^{-37}), and the recursion relation is used to obtain the $j_\ell(\alpha)$, $\ell=n-2, \dots, 0$. Here n is chosen as 30 for $\alpha \geq 1.0$, and depends on α for $\alpha < 1$. The backward recursion, starting with these arbitrary choices of high order values, produces a set of values which satisfies the recursion relation but does not fulfill the additional condition $j_0(\alpha) = \sin(\alpha)/\alpha$. The series of values is normalized to this value of j_0 , which gives a correct representation of the $j_\ell(\alpha)$ for $\ell < n$, since errors introduced by the arbitrary choice of $j_n(\alpha)$ and $j_{n-1}(\alpha)$ damp out if $j_{n-1}(\alpha)$ is truly small compared to the values of $j_\ell(\alpha)$ for the range of interest of ℓ .

The basic integral $A_{00}^+(\alpha, \lambda)$ is calculated by a repeated 10-point gaussian quadrature routine, in which the number of points used is made to depend on α . For $\alpha \leq \pi$, 10 points are used. For $\alpha > \pi$, $n \times 10$ points are used, where n is the integer part of α/π . This procedure ensures that the integrand is slowly-varying between integration points.

Since P_0 and P_1 kernels for both para- and ortho-hydrogen more than fill the memory for any reasonable energy mesh, the ortho-hydrogen kernels are stored on a scratch tape as they are calculated by the routines $B\phi$ and $XB\phi$. These are supplied information one word at a time; when 100 have been collected, the block is written on tape. Reading the information back is controlled by routines BI and XBI, which supply one word at a time to the calling program, reading in a block of 100 whenever necessary. These routines were mandatory for the 7090 to reduce the amount of tape used and the time spent in writing and reading tapes; they are probably less necessary for the 7044 but have been left in to avoid reprogramming.

III. Approximations and Checks

The simpler expressions for $\sigma_p(E, E_0, \mu)$ and $\sigma_o(E, E_0, \mu)$ given by (1a) and (2a) are used whenever $\kappa^2/8mw < E_{c2}$ provided the initial energy $E_0 < E_{c1}$. A value of $E_{c2} = .01$ has joined these expressions smoothly to the regular expressions (1) and (2) for $E_{c1} = 0.3$ ev. Higher values of E_{c2} , up to 0.1 say, should be tried. E_{c1} should probably not be any greater than 0.3, since expressions (1a) and (2a) do not apply above the first vibrational level.

The number of vibrational levels treated is now given by the smallest integer n (one greater than the number of vibrational quanta) satisfying

$$n > \frac{\sqrt{E_0 kT} + 2/3 E_0}{3}$$

$$1 \leq n \leq 5.$$

The largest number of rotational levels allowed is now set to 15, which allows for initial energies up to 1.0 ev. The $A_{n,l}^{\pm}$ are calculated for n vibrational levels and 15 rotational levels always; the sums in (1) and (2) being truncated in l (when no further significant contribution is made) as follows: for $n = 1$, l goes from 1 to 3 always, and stops when either l reaches 15 or the argument of the ortho exponential term (since this peaks at a higher l than the para- term) is increasing and the term itself is less than 10^{-7} . For $n > 1$, the sum is truncated as above for any value of l from 2 to 15.

For $\lambda \leq 2$ the $A_{n,\ell}$ are calculated with eq. (7) using terms in v up to the v_{\max} for which $(\lambda)^v/v! \leq 10^{-4}$. A cutoff value of 10^{-4} produces double-differential cross sections differing in the third or fourth place from those calculated with a cutoff of 10^{-3} . A cutoff value of 10^{-4} has so far been found to be consistent with $v_{\max} \leq 10$ for a maximum energy of 1 ev.

A consistency check was made by comparing the $A_{n,\ell}$ for $\lambda = 2 \pm 10^{-3}$, so that the expansion and recursion techniques were used for very nearly equal arguments. The two methods produced answers well within the expected agreement. Hand checks of both methods were also made.

The spherical bessel functions, $j_\ell(\alpha)$, used in Eqs. (1a) and (2a) and in the expansion form of the $A_{n,\ell}$ for $\lambda \leq 2$ have been calculated several ways to check the methods used. The forward recursion relation was found to break down for various ranges of the argument. The backward recursion technique gives sufficient accuracy over the ranges of argument encountered (the ranges are limited by $\lambda \leq 2$ and $\alpha^2/8m\omega \ll E_{c2}$).

IV. Proposed Changes

Should it ever be necessary to generate kernels with more than about 80 energy points, data that is now left in core would have to be stored on tape for later use. The P_1 para kernel could easily be put on tape, releasing about 6400 locations. After punching the P_0 para kernel and calculating total P_0 cross sections, the P_1 kernel could be read back

into the location occupied by the P_0 kernel, punched, and have total P_1 cross sections calculated. The ortho kernels could then be treated the same way.

The basic calculation could be speeded up considerably if a simple method of predicting the number of terms needed in l in Eqs. (1), (1a) and (2), (2a) were available; this would eliminate unnecessary calculations of the $A_{n,l}$.

The current version of the code calculates cross sections for liquid hydrogen only. The basic subroutine LHK could be rewritten using the formulation given in reference (1) in terms of the Clebsch-Gordon coefficients which allows for treating molecular hydrogen at much higher temperatures.

The code could easily be modified to calculate molecular deuterium cross sections, as given in reference (1).

An additional calculation option might be added to calculate

$$\frac{d\sigma(E)}{d\Omega} = \int_0^{E_{\max}} dE' \frac{d^2\sigma(E \rightarrow E', \mu)}{d\Omega dE'} .$$

The coding to do this would be the same as the kernel generating section of the code, with the angle integration deleted. It is not possible to combine this sort of calculation with a kernel calculation since the double-gaussian quadrature used for the kernels does not produce the same set of angles for various final energies with fixed initial energies.

V. Input

Various constants are built into the program, and are set in the subroutines SETLHK. They are: $\hbar^2 = 0.433192 \times 10^{-30} (\text{ev} \cdot \text{sec})^2$,

$\omega = 0.54617$ ev, proton mass = 1.67243×10^{-24} gm, the equilibrium atomic separation $a = 0.75 \text{ \AA}$, and the coherent and incoherent scattering amplitudes $a_c = 0.0352$ and $a_i = 1.586$.

Card	Format	Name	Description
1	13A6, I2	HØLREC,	label, columns 73-78 are output kernel card label.
		IP	IP > 0 to print double differential data during kernel calculation. IP = 0 to eliminate this printing.
2	3I10, 4E10	ID, NE, NA, T, BARNs, EC1, EC2	ID = numeric identification NE = number of energies NA = number of angles T = Temperature in ev divided by 0.0253 BARNs = bound hydrogen cross section (81.6 barn) EC1 = highest energy at which (1a) and (2a) may be used (0.3). EC2 = value of $\kappa^2/8m\omega$ below which (1a) and (2a) may be used if $E_0 < EC1(0.01)$.
3	I10, E10	IBUG, AMULM	IBUG = 0 for kernel calculation = 2 for double-differential cross section calculation AMULM = limit of absolute value of division point θ of angular integration range for double-gaussian quadrature (see Eq. (8)). AMULM set to 0.9 if left blank.

Section A If IBUG = 0, continue input from Section B

4a	2I10	NMUS, NES	NMUS = number of angles for double-differential calculation NES = number of energies for double-differential calculation.
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<u>Card</u>	<u>Format</u>	<u>Name</u>	<u>Description</u>
5a	2E10	D,M	NMUS values of angles, expressed as D degrees and M minutes (one angle per card).
6a	7E10	E	NES energies. The last (highest) energy is used as initial energy, and double-differential cross sections from this energy to all the others at all the angles are calculated.

Return to card 4a for next problem input.

Section B (IBUG=0)

if $NA > 0$ it must be 15, in which case a set of 15 gaussian weights and angles are supplied by the code for the angular integrations. Skip to card 6b.

if $NA < 0$, a double-gaussian quadrature is to be used, with $N = -NA$ points ($N \leq 7$) in each of the two halves of the range, with the additional input of cards 4b and 5b.

4b	7E10	AV	N values of angles for double-gaussian quadrature.
5b	7E10	AWV	N values of weights for double-gaussian quadrature ($\sum \text{weights} = 1.0$).
6b	6E12	E	NE values of energy for kernel calculation.

Return to card 1 for next problem input.

ACKNOWLEDGEMENT

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